OST TECHNICAL PROGRESS REPORT FOR FY2001
MATERIALS EVALUATION/ CFD MODELING TEAM
CLEAN AIR TECHNOLOGY DIVISION
Team Leader : Mahendra Mathur

PROJECT 1. HIGH TEMPERATURE MATERIALS EVALUATION:

TEAM: William O'Dowd, Mahendra Mathur, Mark Freeman, Clement Lacher

DESCRIPTION:

This project continues activities with numerous external organizations that are conducting advanced material's R&D to support the Indirect-Fired Cycles Program and Advanced Research & Technology Development Program. These programs have emphasized development of high-temperature ceramic and alloy materials for heat transfer applications, such as slag screens for high-temperature advanced furnaces, and crosscutting applications, such as filters**.** New materials are needed for applications in advanced power systems because of the higher operating temperatures and the severe environment. A new variety of materials have been developed and appear to be viable candidates. Several of these materials have been tested in different environments and different test equipment as well as on probes in operating power plants, but much more testing is required. Tests in boilers are expensive and are limited in operating conditions, such as temperature. As part of a planned testing program, new materials and advanced coatings will be tested in the pilot-scale coal-burning facilities at NETL (e.g., in the Combustion and Environmental Research Facility (CERF)) and the combustion and hot gas filter facilities at the University of North Dakota's Energy and Environmental Research Center (EERC).

The CERF evaluations are valuable because some researchers under the FE/Oak Ridge-funded projects do not have ready access to pilot-scale facilities and have only used laboratory muffle furnaces (with ash manually applied to surfaces) that do not realistically simulate actual combustion environments. The CERF tests allow verification of these muffle furnace tests and various thermochemical equilibrium model predictions.

RESEARCH OBJECTIVES:

Several new materials systems are potentially applicable to coal-fired combustion. However, because of limited property characterization in actual coal combustion environments, additional research to prove their suitability is warranted. The objective of this research effort was to complete the long duration testing (100-hours) of various promising materials and their components in an actual coal combustion environment using NETL's CERF.

LONG TERM GOALS / RELATIOHSHIP TO NETL's PRODUCT LINE(S):

This research directly supports the Office of Fossil Energy's Indirectly-Fired Cycles Program and Advanced Research & Technology Development Program. New materials are needed for applications in advanced power systems because of the higher operating temperatures and the severe environment. The planned CERF testing directly supports the Fossil Energy Materials

Program and materials' R&D studies conducted at Oak Ridge National Laboratory (ORNL).

Longer term goals are to evaluate the behavior of numerous new materials (and advanced coatings) behavior in realistic fossil fuel composition environments, compare their behavior in different test stands, test at several appropriate temperatures, and relate the results to utility applications.

SUMMARY OF ACCOMPLISHMENTS:
The following four tasks were conducted in the materials project in FY01.

Task1 - McDermott Project. In this task metal welds are currently being exposed in the Ohio Edison Niles Plant in Ohio (high sulfur coal, reheat super heat temperature of 1100 ^{o}F). The samples will be monitored after 1, 3, and 5 years. The last inspection was in April 2000, and the next one is scheduled for April 2002. The same samples are being exposed in NETL's 500 lb/hr unit.

Task 2 - Collaboration with Argonne National Laboratory. Conduct materials evaluation tests on alloys supplied by Argonne while co-firing coal and biomass in the CERF.

Task 3 - Collaboration with West Virginia University. Thermal and mechanical properties of samples obtained from McDermott were conducted.

RESULTS:

In FY01, several probe designs were evaluated for ORNL's dedicated materials tests in the CERF. Although our Inconel 600 probe design worked satisfactorily, the researchers at ORNL thought that silicon from the Inconel 600 might adversely affect the some samples, such as ODS alloys, because of their proximity to Inconel 600 plates. A ceramic swing design was proposed to alleviate this problem. But, unfortunately, the ceramic shattered while cooling down. This happened two times, so the probe design was abandoned. The group decided to fabricate the probe out of Inconel 601, which does not contain silicon. This required using custom-made Inconel 601 bars for the probe. The cost of such a probe was prohibitive, however, because the vendor would have to make the Inconel 601 especially for us. Fortunately, ORNL suggested the use of Haynes HX (Hastelloy). One of ORNL's contractors, Specialty Metals, had scrap Hastelloy plates, which they were willing to ship to us. We cut the plates into bars and fabricated the probe. This effort consumed a great deal of time, and, as a result, the testing of the samples in the CERF was delayed. Some results are shown in Figure 1.

PROJECT 2. COMPUTATIONAL FLUID DYNAMICS MODELING OF COMBUSTORS:
TEAM: Mahendra Mathur, Mark Freeman, Dinesh Gera (Fluent) and Allen Robinson (CMU)

DESCRIPTION:
The computer simulations of coal-fired combustors are an economically efficient tool for evaluating the design and control strategies to improve energy (fuel) efficiency, process stability, and emissions control. The current state-of-the-art technology is now capable of solving the complex interdependent processes like fluid flow, turbulence, particle trajectories, heat transfer, soot generation, and heterogeneous and homogeneous chemical reactions involved in fossil fuel combustion. However, the complete description of the chemistry of devolatilization and char oxidation is still based on kinetically simple empirical models that do not account for the chemical structure and complicated physics of the process. A recent sensitivity study of a CFD-based coal combustion model has shown that uncertainty in the devolatilization and oxidation parameters has a dominant effect on unburned carbon in model predictions (Jones et al., 1999). The purpose of this study is to perform some exploratory simulations in a lab/pilot-scale combustor that examines the effects of fuel shape, size, and injection location on unburned carbon and NO_x emissions.

The mathematical model is based on the commercial CFD code, FLUENT, where the gas flow is described by the time-averaged equations of global mass, momentum, enthalpy, and species mass fractions. The particle-phase equations, formulated in Lagrangian form, and the coupling between phases are introduced through particle sources in the Eulerian gas-phase equations. The standard k-□ turbulence model, two-mixture-fraction probability density function (PDF), and the discrete ordinate radiation models are used in the present simulations. The coal devolatilization is simulated using the two-competing-rates Kobayashi model, and the char oxidation is modeled as the kinetics-controlled surface reaction. The biomass devolatilization is incorporated using an Arrhenius-type, first-order kinetic rate model. The biomass char oxidation is controlled by diffusion-limited surface reaction, and it is modeled as a constant density process. The standard FLUENT code has been updated with the modified char oxidation sub-models for coal and biomass via an externally defined user function.

CERF engineers are working together with FLUENT to develop and validate comprehensive combustion sub-models for cofiring biomass in pulverized coal boilers. This fundamental research is focussed on developing strategies for NO_x reductions by reburning highly volatile, moist biofuels in utility boilers. Minimizing the unburned carbon in ash is one of the factors used to evaluate biomass fuels for utility boilers. Accurate prediction of unburned carbon in a highly fluctuating environment, like that found in utility boilers, requires the use of advanced carbon burnout kinetic models in CFD simulations.

REAEARCH OBJECTIVES:
The research objective of this study is to develop a 3-dimensional combustor model for biomass co-firing and reburning applications using the FLUENT CFD code.

LONG TERM GOALS / RELATIONSHIP TO NETL□s PRODUCT LINE(S):
The long term goal is to develop and validate specialized CFD sub-models for predicting unburned carbon and NO_x emissions from co-firing or reburning of biomass in pc full-sized utility boilers. These sub-models can be used as a component in the virtual demonstration of power

plants. Also, NETL will develop an extensive CFD and experimental database for different coals. This project supports the mission of two product lines, viz., Vision 21 and Advanced Power Systems.

SUMMARY OF ACCOMPLISHMENTS:

- Integrated moisture submodel with our recently developed CBK model
- Developed and tested a model to include the effect of moisture on coal and biomass combustion characteristics on a full-scale 150-MW GE-EER boiler
- Tested the robustness of an integrated moisture and CBK submodel with extreme levels of moisture fractions in the biomass to predict the flame lift-off in a pilot scale combustor
- It was inferred that the CFD simulations could be used to predict the burnout of different biomass particle sizes. It can assist in determining the optimum biomass size that can be successfully used in coal and biomass cofiring in industrial boilers
- Developed a model to incorporate heat conduction effects in radial and axial directions
- Created an animation to depict the particle orientation during its trajectory in a combustor
- Created an animation to show the effect of moisture on flame characteristics inside the CERF combustor
- Created an animation to show the flow characteristics inside an industrial boiler

RESULTS:

In FY01, several CFD simulations were conducted to investigate the effects of moisture in the feed, particle injection locations, and flow parameters on carbon burnout and NO_x inside a 150-MW GE-EER industrial boiler. Various simulations were designed to predict the suitability of biomass cofiring in coal combustors and to explore the possibility of using biomass as a reburning fuel to reduce NO_x. Some additional CFD simulations were also conducted on the CERF combustor to examine the combustion characteristics of pulverized coal in enriched O_2 and CO_2 environments. Most of the CFD models available in the literature treat particles as point masses with uniform temperature inside the particles. This isothermal condition may not be suitable for larger biomass particles. To this end, a stand-alone program was developed from first principles to account for heat conduction from the surface of the particle to its center.

This study involved the development of FLUENT subroutines for biomass combustion and cofiring using available experimental data and first principles mathematical models that provide accurate estimations of kinetic and CFD model parameters for devolatilization and diffusion-controlled char burnout. Two sets of drying functions have been developed to include the effect of moisture present on the surface of coal or biomass and embedded in the char, which is typical of the conditions found in low-rank coals. The effect of moisture on the surface of the coal or biomass particle is incorporated using a droplet vaporization model in FLUENT. The evaporation of moisture embedded in char is included via a surface reaction in a novel way that accounts for char burnout due to steam gasification. Another key concern in developing an accurate model for biomass combustion is accounting for significant asphericity in biomass char particles, which plays a key role in char burnout. To this end, an enhancement factor that accounts for the large length-to-diameter aspect ratio in the burning of biomass particles has been explicitly derived for

FLUENT computations.

In FY01, we examined a number of interesting exploratory CFD simulations related to the CERF pilot-scale combustor geometry and to a T-fired industrial boiler. The simulations were conducted to examine the effects of biomass particle size and residence time on carbon burnout (see Figure 2.) . Interestingly, despite ten times larger biomass (switch grass) particle sizes relative to coal, blending biomass with coal in the boiler actually reduced the unburned carbon in the ash. This phenomenon can be attributed to the high volatile content of the switch grass. A few additional exploratory CFD simulations were performed on the CERF combustor to examine the effect of O_2 and CO_2 on NOx emissions. From the preliminary results, a reduction of 39% in NO_x (on a lb/MMBtu basis) was observed when compared with the combustion of coal in air.

Over the next year, it is expected that 3-D CFD simulations will be conducted for at least three full-scale utility boilers to asses the design and operational issues. The validated 3-D CFD model, in conjunction with the engineering guidelines for allowable biomass type, particle size, and moisture, will also be related to biomass fuel handling and process economics work for various power plant equipment and burner design and injection schemes. This CFD modeling, with new biomass cofiring routines, will represent a new capability for commercial software and should nicely complement goals related to the co-firing of opportunity fuels and the longer-term need to couple and integrate 3-D CFD simulations with plant-modeling software for dynamic simulations. Information from the full-scale demonstrations will also provide feedback for refinement of the CFD model and insight into design and operational issues that are important for planning future utility biomass cofiring demonstration projects.

PUBLICATIONS and PRESENTATIONS:

Gera, D., Mathur, M., Freeman, M., and O□Dowd, W. (2001). Moisture and char reactivity modeling in pulverized coal combustors. Combustion Science & Technology (to be published).

Gera, D., Mathur, M., Freeman, M., O□Dowd, W. J., Walbert, G., and Robinson, A. (2001). Computational fluid dynamics modeling for evaluating design and operational issues for biomass cofiring in coal-fired boilers. 5th International Biomass Conference of the Americas, Orlando, FL, September 17-21, 2001.

Gera, D., Mathur, M., Freeman, M., and O□Dowd, W. (2001). Effect of moisture and variable char reactivity on biomass/coal cofiring units. 2001 Joint AFRC/JFRC/IEA Combustion Symposium, Kauai, HI, September 9-12, 2001.

Gera, D., Mathur, M., Freeman, M., and O□Dowd, W. (2001). On the CFD analysis of 500,000 Btu/hr combustor using enriched O_2 and recycled flue gas. 2001 Joint AFRC/JFRC/IEA Combustion Symposium, Kauai, HI, September 9-12, 2001.

Gera, D., Mathur, M., Freeman, M., Walbert, G., and Robinson, A. (2000). Computational fluid dynamics modeling for biomass cofiring design in pulverized coal boilers. Bioenergy 2000, Buffalo, NY, October 16-20, 2000.

Gera, D., Mathur, M., and Freeman, M. (2001). Moisture and char reactivity modeling in pulverized coal combustors. Fluent Spring Newsletter.

Mathur, M. P., Freeman, M., O Dowd, W., Lacher, C., and Walbert, G. (2001). High temperature testing of advanced materials in actual coal combustion environments. The Fifteenth Annual Conference on Fossil Energy Materials, Knoxville, TN, April 25-27, 2001.

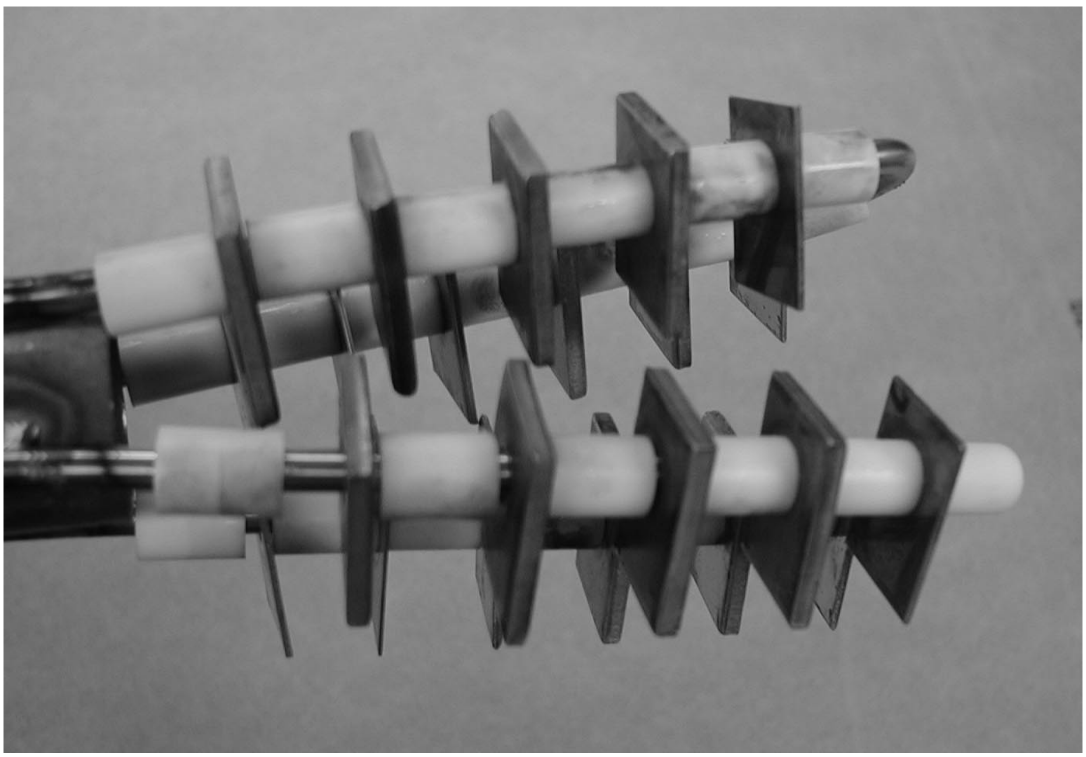

Figure 1. Hastelloy X Probe with alumina spacers -samples exposed at 1500-1600 ^{o}F during the CERF test

Typical Biomass Particle Burnout

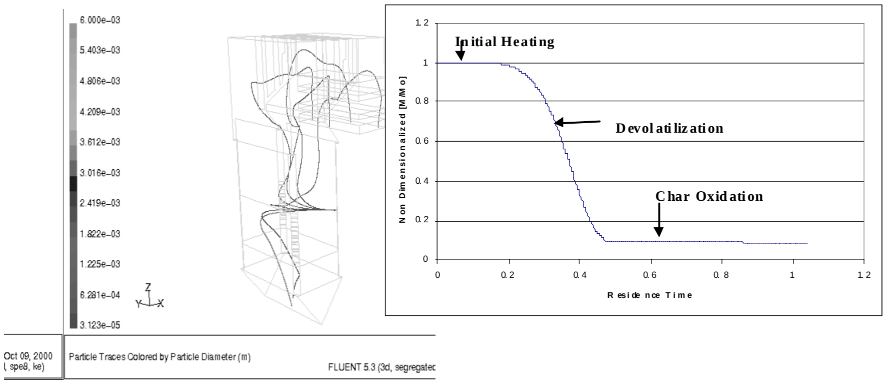

Figure 2. Calculated biomass particle trajectories and particle burnout as a function of residence time